

Fixed Energy R-separation for Schrödinger equation

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Abstract

We extend the classical approach of the R -separation of the Laplace equation $\Delta\psi = 0$ (as a null eigenvalue problem) to the general steady state Schrödinger equation including cases with a scalar potential V and the energy is a fixed constant.

Keywords: Variable separation; Schrödinger equation; Laplace equation; R-separation.

1 Introduction

Let us consider the Schrödinger equation

$$-\frac{\hbar^2}{2}\Delta\psi + (V - E)\psi = 0, \quad (1.1)$$

on a Riemannian manifold Q with metric tensor \mathbf{G} of any signature. According to Moon and Spencer [15, 16, 17], if the ansatz

$$\psi = R \prod_i \phi_i(q^i),$$

where R is a suitable function of the coordinates and each ϕ_i is a function of the corresponding coordinate q^i only, permits to split equation (1.1) into n separated ODE's, then this equation is said to be *R-separable*. We are interested in the following question: under which conditions on the metric \mathbf{G} , the potential V and the value of the energy E is this ansatz successful?

Usually, in the literature [15, 16, 17, 10, 13, 8, 7], authors require that R -separable solutions for Schrödinger or Helmholtz equations exist for all possible eigenvalues E . In the present paper we study the more general theory in which R -separation occurs for a single eigenvalue E , as in the Laplace equation, where the only eigenvalue is $E = 0$. We call this theory *fixed energy R-separation* (*FER-separation*). As a result, we shall see that FER-separation enlarges the number of classes of separable coordinates. First of all we analyse the definition of FER-separation, showing that the functions ϕ_i must depend on a suitable number of

parameters (c_α) in order to satisfy a completeness condition (Definition 19). According to this definition, we will provide a criterion for testing if FER-separation occurs in a given coordinate system (q^i) (Theorem 30): we shall see that a necessary condition is that coordinates be orthogonal and *conformal separable* (as defined in [4]). Then, we give necessary intrinsic conditions for the existence of FER-separable coordinates based on conformal Killing tensors (Proposition 37). Furthermore, ODEs whose integrations provide R -separated solutions of (1.1) are deduced and the associated second order commuting operators are determined. In such a way, we see that our definition of R -separation is equivalent, when restricted to the Laplace equation, to the definition of orthogonal separable coordinates given by Kalnins and Miller [9] involving a set of operators constructed from a Stäckel matrix. Indeed, the R -separation of Laplace equation is characterized in [9] by means of *conformal symmetry operators*. We remark that in our approach, both the orthogonality and the existence of a related Stäckel matrix are proved and not assumed.

Also the intermediate results, the “tools” used for proving Theorem 30, appear to be quite interesting by their own: they are (i) a geometric interpretation of the additive separation of variables in a single null PDE of any order, (ii) three criteria for additive separation of such a PDE, which extend those given for the null Hamilton-Jacobi equation in [4], both exposed in Section 3. This geometrical approach is quite general and easily adapted for dealing with fixed energy separation and FER-separation of other PDE’s of physical interest, like time-dependent Schrödinger equation or Schrödinger equation with a vector potential. For instance, as a straightforward application of the method, we get that, on an Einstein manifold, ordinary separation for a single value of E of (1.1) only occurs in the coordinates allowing separation for all admissible values of E (this is well-known for the Laplace equation, which on Einstein manifolds is separable in the same coordinates separating Helmholtz equation). In other words, studying the fixed energy case of ordinary separation is not so interesting, since in the most common cases we do not get any new coordinate system, while for FER-separation the class of possible coordinates is definitively bigger. This is explain the importance of FER-separation, whose theory, even if applied to Laplace equation till the 19-th century, needs a precise mathematical foundation.

2 From multiplicative R -separation to additive separation

The link between R -separation of (1.1) and additive separation of a suitable PDE depending on \mathbf{G} , V , R , and E is obtained via the usual (see for instance [10]) substitutions,

$$u = \ln \phi \tag{2.1}$$

$$\psi = R\phi. \quad (2.2)$$

We recall that the Laplace-Beltrami operator $\Delta = g^{ij}\nabla_i\nabla_j$ on a n -dimensional Riemannian or pseudo-Riemannian manifold (Q, \mathbf{G}) with contravariant metric tensor $\mathbf{G} = (g^{ij})$ in local coordinates has the form

$$\Delta\psi = g^{ij}\partial_{ij}^2\psi - \Gamma^h\partial_h\psi. \quad (2.3)$$

where Γ^h are the *contracted Christoffel symbols*, defined as

$$\Gamma^h = g^{ij}\Gamma_{ij}^h, \quad \Gamma_k = g_{kh}\Gamma^h. \quad (2.4)$$

Proposition 1. *There is a one to one correspondence between the solutions of (1.1) of the form $\psi = R\prod_i \phi_i(q^i)$ and the additively separated solutions $u = \ln \phi$ of*

$$g^{ij}u_i u_j + g^{ii}u_{ii} - \hat{\Gamma}^i u_i + \frac{2}{\hbar^2}E - U = 0, \quad (2.5)$$

where $u_i = \partial_i u$, $u_{ii} = \partial_{ii}^2 u$, U is the modified potential

$$U = -\left(\frac{\Delta R}{R} - \frac{2}{\hbar^2}V\right), \quad (2.6)$$

and

$$\hat{\Gamma}^i = g^{ij}(\Gamma_j - 2\partial_j \ln R). \quad (2.7)$$

Proof. By inserting (2.2) in (1.1) for a real function $R \neq 0$ on Q , we see that (2.2) is a solution of (1.1) if and only if ϕ satisfies

$$R\Delta\phi + 2\nabla R \cdot \nabla\phi + \left(\frac{2}{\hbar^2}R(E - V) + \Delta R\right)\phi = 0. \quad (2.8)$$

which is equivalent to

$$\Delta\phi + 2\nabla \ln R \cdot \nabla\phi + \left(\frac{2}{\hbar^2}E - U\right)\phi = 0, \quad (2.9)$$

where U is given by (2.6). Then, let us perform the substitution (2.1) and let us denote the partial derivatives of u by $u_i = \partial_i u$, $u_{ij} = \partial_{ij}^2 u$, $u_{ijk} = \partial_{ijk}^3 u$, etc. Since u is additively separated, we get $u_{ij} = \delta_j^i u_{ii}$. Moreover, by (2.1) we have

$$\partial_i\phi = u_i\phi, \quad \partial_{ii}^2\phi = (u_{ii} + u_i^2)\phi, \quad \partial_{ij}\phi = u_i u_j\phi \quad (i \neq j). \quad (2.10)$$

Therefore, by inserting (2.10) in (2.9), due to (2.4), we get

$$(g^{ij}u_i u_j + g^{ii}u_{ii} - \hat{\Gamma}^i u_i + \frac{2}{\hbar^2}E - U)\phi = 0.$$

Hence, since $\phi \neq 0$, ϕ is a multiplicatively separated solution of (2.9) if and only if u is a separated solutions of (2.5). \square

Remark 2. Although Eqs. (2.8) and (2.9) admit the same solutions for any choice of $R \neq 0$, they are deeply different from the point of view of separability: equation (2.9) is treated in a natural way as an eigenvalue problem and its separation for all the eigenvalues $\frac{2}{\hbar^2}E$ leads to R -separation theory as developed by Moon and Spencer [15, 16] and by Kalnins and Miller [8, 7, 13, 11]. On the contrary, in (2.8) the energy constant E is multiplied by the function R and E cannot be considered as a differential operator eigenvalue: in (2.8) E is a fixed parameter incorporated into the differential operator and the solutions are the eigenfunctions of the null eigenvalue only. Its separation must be treated in a way similar to the separation for Laplace equation [15, 9]. The difference between these two view points is subtle but relevant (see also [5] about the correspondence between the quantum-mechanical description of hydrogen atom and the harmonic oscillators). Of course, also Eq. (2.9) can be read as a null eigenvalue problem by including the constant E into the potential function $U_E = \frac{2}{\hbar^2}E - U$. We adopt this last interpretation of (2.9) to define Fixed Energy R -separation (FER-separation) in Section 4. In this approach the function R plays the same role of the potential V and the metric tensor (g^{ij}) : Eq. (2.9) is a PDE defined by \mathbf{G} , V , R and E . By imposing that (2.9) admits a complete family of separated solutions ϕ , in a meaning we will make precise later, we determine differential conditions on \mathbf{G} , V , R and E .

Remark 3. The change of unknown function (2.1) relates multiplicative and additive separation of any PDE, both in the case in which we are dealing with a single null PDE or with an eigenvalue problem. In the resulting equation (2.5) the parameter E admits two interpretations as in equation (2.9): it can be considered as an internal parameter of the equation (FER-separation) or as an integration constant (classical R -separation).

3 Geometry of the additive separation for a null PDE of order l

We provide the geometric framework and the geometric characterization of the separation of variables (SOV) for a null PDE of arbitrary order l , extending the results of [4] (concerning the Hamilton-Jacobi case only) and of [2] (dealing with ordinary separation only). The main tool is the theory of separable connections as introduced by Benenti [1]. As in the case of the Hamilton-Jacobi equation with a fixed value of the energy, two different (but in a sense equivalent) definitions of separable solutions are given. Each of them is useful to prove different criteria of existence of a separable solution in a given coordinate system.

3.1 Separable connections

Let $M = Q \times Z \rightarrow Q$ be the trivial vectorial bundle with fiber Z over Q , where Q is a n -dimensional manifold with coordinates (q^i) ($i = 1, \dots, n$) and Z is a N -dimensional vector space (over \mathbb{R} or \mathbb{C}) with coordinates (z^A) ($A = 1, \dots, N$).

We call *connection* on M a regular distribution (in the Frobenius sense) \mathcal{C} on M of rank n and transversal to the fibers: $\mathcal{C} : x \mapsto \mathcal{C}_x \subset T_x M$ with $\dim \mathcal{C}_x = n$ and $\mathcal{C}_x \cap T_x Z = \{0\}$.

A vector field $X \in \mathcal{X}(M)$ is horizontal if $X(M) \subset \mathcal{C}(M)$ i.e., if $X(x) \in \mathcal{C}_x$. Locally a connection \mathcal{C} is spanned by the n horizontal vector fields, called the *generators* of \mathcal{C}

$$D_i = \frac{\partial}{\partial q^i} + C_{iA} \frac{\partial}{\partial z^A},$$

where C_{iA} are functions on M called *coefficients* of the connection. A connection is *integrable* (in the Frobenius sense) if for any point $P \in M$ there exists a unique integral manifold (i.e., a n -dimensional immersed submanifold tangent to each D_i) passing through P . By the Frobenius theorem and the particular form of the generators, we get that

Proposition 4. *A connection generated by the vector fields (D_i) is integrable (in the Frobenius sense) if and only if $[D_i, D_j] = 0$.*

If \mathcal{C} is integrable, then there exists a foliation \mathcal{L} of M made of integrable n -dimensional manifolds of \mathcal{C} . Since \mathcal{C} is a transversal distribution, the integral manifolds are locally described by $z_A = F_A(q^i, c_B)$ where (c_B) are real parameters ($B = 1, \dots, N$) satisfying the completeness condition

$$\det \left[\frac{\partial z_A}{\partial c_B} \right] \neq 0.$$

The functions F_A are solutions of the first-order differential system of PDE on Q

$$\frac{\partial z_A}{\partial q^i} = C_{iA}(q^i, z_A).$$

It follows that

Proposition 5. *The connection generated by the D_i is integrable if and only if the corresponding system of PDE is completely integrable.*

Let S be a $N - 1$ -dimensional submanifold of M . We say that a distribution \mathcal{C} is *reducible* on S if when it is restricted to the points of S it gives rise to a distribution \mathcal{C}_0 on S . We have that

Proposition 6. *A distribution is reducible to a submanifold S if and only if its generators D_i are tangent to S .*

If F is a function on M such that equation $F = 0$ implicitly defines the submanifold S , then \mathcal{C} is reducible to $F = 0$ if and only if $D_i F|_S = 0$ or, equivalently, $D_i F = \Lambda F$ for a suitable function Λ on M .

Remark 7. If a connection \mathcal{C} is integrable and reducible as a distribution to S , then the foliation $\mathcal{L} = (L_{c_A})$ on M made of integral manifolds of \mathcal{C} can be restricted to a foliation \mathcal{L}_S on S made of integral manifolds of \mathcal{C} , whose labels (c_A) belong to a suitable $N - 1$ -dimensional submanifold \mathcal{P} of \mathbb{R}^N . Up to a new parametrization of the (c_A) , we can assume without loss of generality that \mathcal{P} is defined by $c_N = 0$ and \mathcal{L}_S is described by the $N - 1$ parameters $(c_\alpha) = (c_1, \dots, c_{N-1})$.

3.2 Equivalent definitions of additive SOV for a null PDE

Inspired by the approach to the additive separation of Kalnins and Miller exposed in [10] for PDE of the kind $\mathcal{H} = \text{const.}$, we extend the theory in a geometrical way to a single PDE of order l on Q

$$\mathcal{H}(q^1, \dots, q^n, u, u_i, u_{ij}, \dots, u_{ij\dots h}) = 0, \quad (3.1)$$

where $u_i = \partial_i u$, $u_{ij} = \partial_{ij}^2 u \dots$ are the derivatives (up to order l) of the unknown function $u = u(q^i)$, with respect to the coordinates, with $\partial_i = \partial/\partial q^i$. An (additive) *separated solution* of (3.1) is a function of the form

$$u = \sum_{i=1}^n S_i(q^i),$$

where S_i depends on the single variable q^i satisfying (3.1). If we look for additive separated solutions only, Eq. (3.1) reduces to

$$\mathcal{H}(q^1, \dots, q^n, u, u_i, u_i^{(2)}, \dots, u_i^{(l)}) = 0.$$

where $u_i^{(2)} = u_{ii}$ and $u_{ij} = 0$ for $i \neq j$.

Definition 8. Given a PDE (3.1) of order l , the function u^I is a *complete internal separated solution* (internal solution) if: i) u^I is of the form

$$u^I = \sum_{i=1}^n S_i(q^i, c_\alpha), \quad \alpha = 1, \dots, nl;$$

ii) for all (c_α) in a suitable open set of \mathbb{R}^{nl} u^I is a separated solution of (3.1) i.e.

$$\mathcal{H}(q^1, \dots, q^n, u, u_i^I, u_{ii}^I, \dots, u_{ii\dots i}^I) = 0;$$

iii) the following completeness condition holds

$$\text{rank} \left[\frac{\partial u^I}{\partial c_\alpha} \left| \frac{\partial u_i^I}{\partial c_\alpha} \right| \frac{\partial u_{ii}^I}{\partial c_\alpha} \left| \dots \right| \frac{\partial u_{i\dots i}^I}{\partial c_\alpha} \right] = nl.$$

Definition 9. Given the PDE (3.1) of order l , the function u^E is a *complete extended separated solution* (extended solution) if: i) u^E is of the form

$$u^E = \sum_{i=1}^n S_i(q^i, c_a), \quad a = 1, \dots, nl + 1,$$

ii) u^E satisfies (3.1), that is $\mathcal{H}(q^1, \dots, q^n, u^E, u_i^E, u_{ii}^E, \dots, u_{i \dots i}^E) = 0$, for any (c_a) belonging to a suitable nl -dimensional submanifold of \mathbb{R}^{nl+1} or, up to a transformation of the (c_a) , for $c_{nl+1} = 0$; iii) u^E satisfies the following completeness condition for all admissible values of q^i and c_a :

$$\det \left[\frac{\partial u^E}{\partial c_a} \mid \frac{\partial u_i^E}{\partial c_a} \mid \frac{\partial u_{ii}^E}{\partial c_a} \mid \dots \mid \frac{\partial u_{i \dots i}^E}{\partial c_a} \right] \neq 0.$$

Remark 10. An internal complete solution defines a foliation of the submanifold $\mathcal{H} = 0$ in n -dimensional leaves transversal to the fibers of the bundle M , via equations

$$u = u^I, \quad u_i = \partial_i u^I, \quad u_i^{(2)} = \partial_{ii}^2 u^I, \quad \dots \quad u_i^{(l)} = \partial_{i \dots i}^l u^I.$$

Each submanifold is parametrized by the value of the nl parameters (c_a) . Conversely, an extended solution defines a foliation of an open subset of M in n -dimensional leaves via equations

$$u = u^E, \quad u_i = \partial_i u^E, \quad u_i^{(2)} = \partial_{ii}^2 u^E, \quad \dots \quad u_i^{(l)} = \partial_{i \dots i}^l u^E.$$

Each submanifold is parametrized by the value of the nl parameters (c_a) . The foliation is compatible with the submanifold $\mathcal{H} = 0$ in the sense that it is reducible to a foliation of $\mathcal{H} = 0$.

Proposition 11. *In the coordinates (q^i) on Q , there exists an internal solution of the PDE (3.1) if and only if there exists an extended solution of (3.1) in the (q^i) .*

Proof. Let $u^E(q^i, c_a)$ be an extended solution of (3.1). Then, up to a reparametrisation of the (c_a) , we can assume that for all (c_a) with $c_{nl+1} = 0$ the function u^E is a solution of (3.1). Hence, $u^I(q^i, c_a) = u^E(q^i, c_1, \dots, c_{nl}, 0)$ is an internal solution for (3.1) in the same coordinates. Conversely, let $u^I(q^i, c_a)$ be an internal solution of (3.1). Let C_m be the first column in the matrix

$$M^I = \left[\frac{\partial u^I}{\partial c_a} \mid \frac{\partial u_i^I}{\partial c_a} \mid \frac{\partial u_{ii}^I}{\partial c_a} \mid \dots \mid \frac{\partial u_{i \dots i}^I}{\partial c_a} \right]$$

such that the nl -th order minor M_m^I obtained by eliminating this column is different from zero. Such an index m exists because of the completeness condition. We

consider the two cases $m = 1$ and $m > 1$ separately. If $m = 1$, then $u^E = u^I + c_{nl+1}$ is a solution of (3.1) for all (c_a) such that $c_{nl+1} = 0$; moreover, we have that

$$M^E = \left[\frac{\partial u^E}{\partial c_a} \mid \frac{\partial u_i^E}{\partial c_a} \mid \cdots \mid \frac{\partial u_{i\dots i}^E}{\partial c_a} \right] = \left[\frac{\partial u^I}{\partial c_\alpha} \mid \frac{\partial u_i^I}{\partial c_\alpha} \mid \frac{\partial u_{ii}^I}{\partial c_\alpha} \mid \cdots \mid \frac{\partial u_{i\dots i}^I}{\partial c_\alpha} \right]$$

and the completeness condition holds. If $m > 1$, there exist unique $q, r \in \mathbb{Z}$ such that $m - 2 = qn + r$ with $0 \leq r < n$. Thus, the eliminated column contains the partial derivatives w.r.t. (c_α) of $\frac{\partial^k u^I}{(\partial q^j)^k}$ with $k = q + 1$ and $j = r + 1$. Then,

$$u^E = u^I + c_{nl+1} \frac{(q^j)^k}{k!}$$

is a solution of (3.1) for all (c_a) such that $c_{nl+1} = 0$. Moreover, the rank of

$$M^E = \left[\frac{\partial u^E}{\partial c_a} \mid \frac{\partial u_i^E}{\partial c_a} \mid \frac{\partial u_{ii}^E}{\partial c_a} \mid \cdots \mid \frac{\partial u_{i\dots i}^E}{\partial c_a} \right]$$

is maximal. Indeed, in the developing of $\det M^E$ along the last row, the first $m - 1$ addenda are null since $M_h^I = 0$ for $h < m$, as well as those from the $(m + 1)$ -th to the last, because the elements of the last row of M^E with column index greater than m are all null. Hence, being $\det M^E = (M^E)_m^{nl+1} M_m^I = 1 \cdot M_m^I \neq 0$, the completeness condition holds. \square

Definition 12. We say that the null equation $\mathcal{H} = 0$ is *separable* in the coordinates (q^i) if it admits an extended solution or, equivalently, an internal one.

Remark 13. In comparison with the geometric framework introduced in [4] to deal with a null Hamilton-Jacobi equation, the present case presents several differences. First of all, it is not possible to define complete internal or extended solutions without assuming that they are separated; moreover there is not a unique formula transforming an internal into an extended solution. This is a consequence of the fact that the coordinates in the fiber are not all of the same kind, but correspond to derivatives of u of different orders.

3.3 Criteria for additive separation of a null equation

Let us consider fibered coordinates (q^i, z_A) on $M = Q \times Z \rightarrow Q$, where $(z_A) = (u, u_i, u_i^{(2)}, \dots, u_i^{(l)})$, with $i = 1, \dots, n$, $A = 1, \dots, nl + 1$. Let \mathcal{H} be a smooth function on M such that $\mathcal{H} = 0$ is a nl -dimensional submanifold of M . We apply to this case the equivalence of integrability of distributions on vector bundles and complete integrability of normal first-order differential systems, recalled in section 3.1. The following propositions provide necessary and sufficient conditions for the existence of an extended and an internal solution, respectively (see also [4] and references therein).

Proposition 14. *In given coordinates (q^i) on Q , the following statements are equivalent: (i) there exists an extended solution u^E of $\mathcal{H} = 0$; (ii) there exist n functions R_i on M such that the distribution Δ generated by*

$$D_i = \partial_i + u_i \partial_u + u_i^{(2)} \partial / \partial u_i + \dots + u_i^{(l)} \partial / \partial u_i^{(l-1)} + R_i \partial / \partial u_i^{(l)} \quad (3.2)$$

is integrable and reducible on the submanifold $\mathcal{H} = 0$, that is

$$\begin{cases} D_i R_j = 0, & \forall j \neq i \\ D_i \mathcal{H}|_{\mathcal{H}=0} = 0. \end{cases} \quad (3.3)$$

Proof. (i) \Rightarrow (ii): Let us assume that a solution $u^E = \sum_i S_i(q^i, c_1, \dots, c_N)$ of $\mathcal{H} = 0$ exists. By the completeness condition, (q^i, c_1, \dots, c_N) are (non fibered) coordinates on M and the n functions on M

$$R_i = \frac{d^{l+1}}{(dq^i)^{l+1}} S_i(q^i, c_1, \dots, c_N)$$

are well-defined. Going back the original coordinates we get functions

$$R_i = R_i(q^i, u, u_i, u_i^{(2)}, \dots, u_i^{(l)}),$$

and by them we construct the vector fields D_i (3.2). The distribution Δ generated by the fields D_i is integrable because the corresponding first order system on M

$$\begin{cases} \partial_i u = u_i \\ \partial_i u_j = \delta_{ij} u_i^{(2)} \\ \dots \\ \partial_i u_j^{(l)} = \delta_{ij} R_j \end{cases} \quad (3.4)$$

is completely integrable. Indeed,

$$u = u^E = \sum_i S_i(q^i, c_A), \quad u_i = \frac{d}{dq^i} S_i(q^i, c_A) \quad \dots \quad u_i^{(l)} = \frac{d^l}{(dq^i)^l} S_i(q^i, c_A)$$

is a complete solution of the PDEs system, which describes a foliation $\mathcal{L}_{(c_A)} = (L_{c_A})$ made of integral manifolds of Δ . Moreover, since u^E is a solution of $\mathcal{H} = 0$ for any (c_A) with $c_{n+1} = 0$, we have $\mathcal{H}(q^i, u^E, \dots) = 0$, that is every point of L_{c_A} belongs to $\mathcal{H} = 0$. Thus, the generators D_i (by construction tangent to every leaf of \mathcal{L}_{c_A}) are tangent to $\mathcal{H} = 0$. Hence, Δ is an integrable distribution reducible to the submanifold $\mathcal{H} = 0$ i.e., conditions (3.3) hold. (ii) \Rightarrow (i). We assume that there exist n functions R_i on M such that the distribution Δ generated by (3.2) is integrable and reducible on the submanifold $\mathcal{H} = 0$, that is (3.2) satisfy (3.3). Hence, the first order PDE system associated with Δ (3.4) is completely integrable, that is there exist $nl + 1$ functions $f_A(q^i, c_B)$ such that $z_A = f_A(q^i, c_B)$ are a complete solution of (3.4) that is satisfy (3.4) and the matrix $(\frac{\partial f_A}{\partial c_B})$ has maximal rank. The form of (3.4) implies that the solution is of separated type:

$$u = \sum_i S_i(q^i, c_B), \quad u_i = \frac{d}{dq^i} S_i(q^i, c_B), \quad \dots \quad u_i^{(l)} = \frac{d^l}{(dq^i)^l} S_i(q^i, c_B)$$

Thus, $u^E = \sum_i S_i(q^i, c_B)$ is an extended solution of $\mathcal{H} = 0$. Indeed, by construction it satisfies the completeness condition. Moreover, being the generators D_i (3.2) tangent to $\mathcal{H} = 0$ by assumption, Δ is reducible to a distribution on $\mathcal{H} = 0$. Then, for any P in $\mathcal{H} = 0$ the connected leaf $L_{(c_A)}$ passing through P is entirely contained in $\mathcal{H} = 0$. Let us consider the submanifold of \mathbb{R}^{nl+1} $\mathcal{P} = \{(c_B) \mid L_{(c_B)} \subset \mathcal{H} = 0\}$. Then, for all $(c_B) \in \mathcal{P}$ u^E satisfies $\mathcal{H} = 0$. \square

Proposition 15. *In a given coordinate system (q^i) on Q the following statements are equivalent: (i) there exists an internal solution $u^I = \sum_i S_i(q^i, c_\alpha)$ of $\mathcal{H} = 0$; (ii) there exist n functions R_i on M such that the distribution Δ generated by the vector fields (3.2) is reducible to a distribution Δ_0 on the submanifold $\mathcal{H} = 0$ and Δ_0 is integrable, that is*

$$\begin{cases} D_i \mathcal{H}|_{\mathcal{H}=0} = 0, \\ D_i R_j|_{\mathcal{H}=0} = 0, \quad \forall j \neq i. \end{cases} \quad (3.5)$$

Proof. (i) \Rightarrow (ii): if there exists an internal solution, then there is also an extended solution in the same coordinates. Hence, by Proposition 14, there are functions R_i satisfying (3.3) and in particular (3.5). (ii) \Rightarrow (i): Being Δ_0 integrable, the manifold $\mathcal{H} = 0$ is foliated by integral manifolds of Δ_0 locally described by solutions of the PDE system (3.4) depending on nl parameters (c_α) with separated form

$$u = \sum_i S_i(q^i, c_\alpha), \quad u_i = \frac{d}{dq^i} S_i(q^i, c_\alpha), \quad \dots \quad u_i^{(l)} = \frac{d^l}{(dq^i)^l} S_i(q^i, c_\alpha)$$

satisfying $\mathcal{H} = 0$. Thus, $u^I = \sum_i S_i(q^i, c_\alpha)$ is an internal solution of $\mathcal{H} = 0$. \square

Theorem 16. *The separation of a null equation $\mathcal{H} = 0$ occurs in a given coordinate system if and only if one of the following equivalent conditions holds:*

1) *there exist n functions $\lambda_i(q, u, u_i, \dots, u_i^{(l)})$ such that the operators (3.2) satisfy*

$$\begin{cases} D_i \mathcal{H} = \lambda_i \mathcal{H}, \\ D_i R_j = 0, \quad \forall j \neq i. \end{cases} \quad (3.6)$$

2) *there exists (locally) a function $\Lambda(q^i, u, u_i, \dots, u_i^{(l)})$ such that the equation $\mathcal{H}/\Lambda = h$ is separable in the ordinary sense, i.e. the operators (3.2) satisfy*

$$\begin{cases} D_i (\mathcal{H}/\Lambda) = 0, \\ D_i R_j = 0, \quad \forall j \neq i. \end{cases} \quad (3.7)$$

3) *the operators (3.2) satisfy*

$$\begin{cases} D_i \mathcal{H} = 0, \\ D_i R_j|_{\mathcal{H}=0} = 0, \quad \forall j \neq i. \end{cases} \quad (3.8)$$

Proof. Condition 1) follows straightforward from (3.3) by applying Hadamard's Lemma: $F|_{\mathcal{H}=0} = 0 \Leftrightarrow F = \lambda\mathcal{H}$. Condition 2) is equivalent to condition 1). Indeed, from (3.3)₁ we get $\lambda_i = D_i \log \mathcal{H}$. Since $D_i D_j = D_j D_i$, we have $D_i \lambda_j = D_j \lambda_i$ and locally there exists a function Λ such that

$$\lambda_i = D_i \log \Lambda.$$

Thus, condition (3.3)₁ becomes $D_i \ln \mathcal{H} = D_i \ln \Lambda$ and, being D_i linear,

$$D_i(\mathcal{H}/\Lambda) = 0.$$

Hence, condition 1) holds iff there exists Λ satisfying (3.7). Condition 3) is a consequence of Proposition 15. Indeed, by applying Hadamard's Lemma to (3.5) and (3.8), we get

$$\exists (\lambda_h), (\mu_{hk}) \mid \begin{cases} D_i \mathcal{H} = \lambda_i \mathcal{H}, \\ D_i R_j = \mu_{ij} \mathcal{H}, \end{cases} \quad \forall j \neq i, \quad (3.9)$$

$$\exists (\nu_{hk}) \mid \begin{cases} D_i \mathcal{H} = 0, \\ D_i R_j = \nu_{ij} \mathcal{H}, \end{cases} \quad \forall j \neq i, \quad (3.10)$$

respectively. We show that (3.9) is equivalent to (3.10). Clearly, (3.10) implies (3.9) by choosing $\lambda_i = 0$. Conversely, we assume that (3.9) holds and we denote by D_i^0, R_i^0 the operators (3.2) and the associated functions R_i satisfying $D_i \mathcal{H} = 0$. moreover we denote by D_i^λ, R_i^λ those satisfying $D_i \mathcal{H} = \lambda_i \mathcal{H}$. Then, we have

$$D_i^0 = D_i^\lambda - \mathcal{F}_i \mathcal{H} \frac{\partial}{\partial u_i^{(i)}}, \quad R_i^0 = R_i^\lambda - \mathcal{F}_i \mathcal{H},$$

where $\mathcal{F}_i = \left(\frac{\partial \mathcal{H}}{\partial u_i^{(i)}} \right)^{-1} \lambda_i$, and by a straightforward calculation we get

$$D_i^\lambda R_j^\lambda = D_i^0 R_j^0 + \mathcal{H} \left[\mathcal{F}_i \frac{\partial}{\partial u_i^{(i)}} (R_j^0 + \mathcal{F}_j \mathcal{H}) + D_i^0 (\mathcal{F}_j) \right].$$

Thus, since $D_i^\lambda R_j^\lambda = \mu_{ij} \mathcal{H}$, there exist functions ν_{ij} such that $D_i^0 R_j^0 = \nu_{ij} \mathcal{H}$. \square

Remark 17. The n additional unknown functions (λ_i) play the role of Lagrangian multipliers. It is remarkable the fact that the n functions (λ_i) can be replaced by a single unknown function Λ .

Remark 18. We recall that the conditions for the separation in the ordinary sense of the equation $\mathcal{H} = h$ are [2, 4, 10]

$$\begin{cases} D_i \mathcal{H} = 0, \\ D_i R_j = 0, \end{cases} \quad (\forall j \neq i). \quad (3.11)$$

4 Definition and criteria for *FER*-separation

By Proposition 1, we can extend the notion of completeness for separated solutions of (2.5) to *FER*-separable solutions of (1.1) in a natural way. However, since \mathcal{H} does not depend on u , but only on its derivatives, the solution of (2.5) is defined up to an inessential additive constant (corresponding to a constant factor for ψ). Hence, in this case we can consider without loss of generality only the $2n$ functions $(z_A) = (u_i, u_{ii})$ as unknowns (see Remark 2.4 in [2]). It follows that in the generators D_i the term $u_i \partial_u$ can be disregarded. Moreover, being the unknown functions $2n$, the number of parameters entering in a complete solution of the null PDE (2.5) is $2n - 1$, according to Section 3.1. Therefore, we define *FER*-separation as:

Definition 19. The Schrödinger equation (1.1) is *FER-separable* in the coordinates (q^i) – called *FER-separable coordinates* for (1.1)– if there exist a value of the energy E and a function R such that Eq. (1.1), admits a solution of the form

$$\psi = R \prod_i \phi_i(q^i, c_\alpha), \quad (4.1)$$

where c_α are $2n - 1$ parameters satisfying the completeness condition

$$\text{rank} \begin{bmatrix} \frac{\partial u_i}{\partial c_\alpha} \\ \frac{\partial v_i}{\partial c_\alpha} \end{bmatrix} = 2n - 1, \quad u_i = \frac{\phi'_i}{\phi_i}, \quad v_i = \frac{\phi''_i}{\phi_i}. \quad (4.2)$$

Remark 20. The meaning of completeness is the following: given R and E allowing *FER*-separation, for any choice of $2n - 1$ numbers $(c_\alpha) = (b_i, k_j)$, $i = 1 \dots n$, $j = 1, \dots, n - 1$, and of a point $q_0 \in Q$, then there exists a unique separated solution ϕ of (2.9) such that $(\frac{\phi'_i}{\phi_i}, \frac{\phi''_i}{\phi_i})_{q_0} = (h_i, k_j)$. Moreover, we observe that in Definition 19 there are no assumptions on the form of the functions ϕ_i (as for instance $\phi_i = e^{b_i q^i}$ with $b_i \in \mathbb{R}$) as in the case of *free separation* of the Schrödinger equation [2].

We apply the third condition of Theorem 16 to study the separation of Eq. (2.5) that is the null equation $\mathcal{H} = 0$ where

$$\mathcal{H} = g^{ij} u_i u_j + g^{ii} u_{ii} - \hat{\Gamma}^i u_i + \frac{2}{\hbar^2} E - U. \quad (4.3)$$

We assume here and in the following that $g^{ii} \neq 0$ for all i . This assumption is obviously fulfilled for a proper Riemannian manifold. This means that we are excluding null coordinates. In our case, we have $l = 2$ and \mathcal{H} independent of u . Hence, both the operators (3.2) and the associated functions R_i do not depend on u :

$$D_i = \partial_i + u_{ii} \frac{\partial}{\partial u_i} + R_i \frac{\partial}{\partial u_{ii}}. \quad (4.4)$$

Since $D_i \mathcal{H} = 0$, the functions R_i have the form

$$R_i(q^i, u_i, u_{ii}) = - \left(\frac{\partial \mathcal{H}}{\partial u_{ii}} \right)^{-1} \left[\partial_i \mathcal{H} + u_{ii} \frac{\partial \mathcal{H}}{\partial u_i} \right]. \quad (4.5)$$

We want to find conditions for which $D_i R_j|_{\mathcal{H}=0} = 0$ ($i \neq j$).

Lemma 21. *The function $D_i R_j$ is a polynomial of second degree in the variables (u_{11}, \dots, u_{nn}) , whose quadratic part is*

$$-2 \frac{g^{ij}}{g^{jj}} u_{ii} u_{jj}, \quad i, j \text{ n.s.} \quad i \neq j. \quad (4.6)$$

Proof. Recalling that $\frac{\partial \mathcal{H}}{\partial u_{ii}} = g^{ii}$, by inserting (4.3) in (4.5), we get

$$R_j = \frac{1}{g^{jj}} [-2 g^{jh} u_{jj} u_h - \partial_j g^{hh} u_{hh} - \partial_j g^{hk} u_h u_k + \partial_j \hat{\Gamma}^h u_h + \hat{\Gamma}^j u_{jj} + \partial_j U].$$

Since R_j and all its partial derivatives contain terms at most linear in the variables (u_{hh}) and being

$$D_i R_j = \partial_i R_j + u_{ii} \frac{\partial R_j}{\partial u_i} - \frac{\partial_j g^{ii}}{g^{jj}} R_i,$$

a straightforward calculation shows that the only term of $D_i R_j$ which is quadratic in (u_{hh}) is (4.6). \square

Proposition 22. *The coordinates (q^i) allowing FER-separation i.e, separation of the null equation $\mathcal{H} = 0$ (2.5) for a suitable R , are necessarily orthogonal.*

Proof. By condition 3) of Theorem 16, the null equation $\mathcal{H} = 0$ is separable if and only if for all $i \neq j$, the functions $D_i R_j$ vanish on the surface $\mathcal{H} = 0$. Since the function (4.3) is linear (u_{hh}) , the equation $\mathcal{H} = 0$ is equivalent to

$$u_{ii} = -\frac{1}{g^{ii}} \left(\sum_{\alpha \neq i} g^{\alpha\alpha} u_{\alpha\alpha} + g^{hk} u_h u_k - \hat{\Gamma}^h u_h + \frac{2}{\hbar^2} E - U \right).$$

Hence, inserting the expression of u_{ii} into $D_i R_j$, we get (by Lemma 21) a quadratic polynomial in the $(u_{\alpha\alpha})$ ($\alpha \neq i$) with quadratic part

$$\sum_{\alpha \neq i} -2 \frac{g^{ij}}{g^{jj}} \frac{g^{\alpha\alpha}}{g^{ii}} u_{\alpha\alpha} u_{jj}, \quad i, j \text{ n.s.} \quad i \neq j,$$

which vanishes if and only if $g^{ij} = 0$ for $i \neq j$. \square

Remark 23. By Proposition 22 coordinates allowing FER-separation of Eq. (1.1) are necessarily orthogonal. However, nonorthogonal R -separation (see [8, 11]) is possible by imposing constraints on the form of some factors ϕ_i : this case, which has been described in [2] for ordinary separation of Schrödinger equation and called *reduced separation*, is not examined in the present paper.

In orthogonal coordinates, (4.3) becomes

$$\mathcal{H} = g^{ii}(u_{ii} + u_i^2) - \hat{\Gamma}^i u_i + \frac{2}{\hbar^2} E - U \quad (4.7)$$

and the functions (4.5)

$$R_j = \frac{1}{g^{jj}}[-2g^{jj}u_{jj}u_j - \partial_j g^{hh}(u_{hh} + u_h^2) + \partial_j \hat{\Gamma}^h u_h + \hat{\Gamma}^j u_{jj} + \partial_j U]. \quad (4.8)$$

In order to write in a shorter way $D_i R_j$ we introduce the following notion ([4])

Definition 24. A *Stäckel operator* S_{ij} is the second order differential operator such that for any $f: Q \rightarrow \mathbb{R}$

$$S_{ij}(f) = \partial_{ij}^2 f - \partial_j \ln(g^{ii}) \partial_i f - \partial_i \ln(g^{jj}) \partial_j f. \quad (4.9)$$

Proposition 25. Equation (2.5) is separable in the orthogonal coordinates (q^i) if and only if

$$\partial_j \hat{\Gamma}^i - \hat{\Gamma}^i \partial_j \ln g^{ii} = 0, \quad (4.10)$$

$$\frac{S_{ij}(g^{hh})}{g^{hh}} - \frac{S_{ij}(g^{kk})}{g^{kk}} = 0, \quad \forall h, k, \quad (4.11)$$

$$S_{ij}(U) g^{hh} - S_{ij}(g^{hh}) (U - \frac{2}{\hbar^2} E) = 0, \quad \forall h. \quad (4.12)$$

Proof. By applying operators (4.4) to the functions (4.8) and using (4.9) we get

$$\begin{aligned} D_i R_j = & \frac{1}{g^{jj}}[(\partial_j \hat{\Gamma}^i - \hat{\Gamma}^i \partial_j \ln g^{ii})u_{ii} + (\partial_i \hat{\Gamma}^j - \hat{\Gamma}^j \partial_i \ln g^{jj})u_{jj} \\ & - S_{ij}(g^{hh})(u_{hh} + u_h^2) + S_{ij}(\hat{\Gamma}^h)u_h + S_{ij}(U)]. \end{aligned} \quad (4.13)$$

We impose that the function $D_i R_j$ vanishes on the surface $\mathcal{H} = 0$ that is for all values of $(u_h, u_h^2, u_{\alpha\alpha})$ with $\alpha \neq i$ and for

$$u_{ii} = u_i^2 - \frac{1}{g^{ii}} \left(\sum_{\alpha \neq i} g^{\alpha\alpha} (u_{\alpha\alpha} + u_\alpha^2) - \hat{\Gamma}^h u_h + \frac{2}{\hbar^2} E - U \right).$$

By inserting the expression for u_{ii} in (4.13) we see that the only coefficient of u_i^2 is $\partial_j \hat{\Gamma}^i - \hat{\Gamma}^i \partial_j \ln g^{ii}$. Thus, (4.10) must hold for any couple of indices $i \neq j$. Then, assuming (4.10), $D_i R_j|_{\mathcal{H}=0}$ becomes (up to a factor g_{jj})

$$\left(\frac{S_{ij}(g^{ii})}{g^{ii}} g^{\alpha\alpha} - S_{ij}(g^{\alpha\alpha}) \right) v_\alpha + \left(S_{ij}(\hat{\Gamma}^h) - \frac{S_{ij}(g^{ii})}{g^{ii}} \hat{\Gamma}^h \right) u_h - \frac{S_{ij}(g^{ii})(U - \frac{2}{\hbar^2} E)}{g^{ii}} + S_{ij}(U) = 0$$

with $v_\alpha = u_{\alpha\alpha} + u_\alpha^2$. By equating to zero the coefficients of v_α , u_h , and of the 0-th order term, we get two conditions equivalent to (4.11), (4.12) and moreover

$$S_{ij}(\hat{\Gamma}^h) - \frac{S_{ij}(g^{ii})}{g^{ii}} \hat{\Gamma}^h = 0.$$

However, this last condition is disregarded being a consequence of (4.10–4.11). Indeed, by (4.10) we get $S_{ij}(\hat{\Gamma}^h) = \hat{\Gamma}^h S_{ij}(g^{hh}) g_{hh}$. \square

Remark 26. If $U - \frac{2}{\hbar^2}E = 0$, i.e., if R satisfies (1.1), then (4.12) is always satisfied.

Proposition 27. *If (q^i) are separable coordinates for (2.5), then the function R is locally determined by integrating equations*

$$2\partial_i \ln R = \Gamma_i - \xi_i(q^i). \quad (4.14)$$

Proof. For $\hat{\Gamma}^i \neq 0$, we have that (4.10) is equivalent to $\partial_j(\hat{\Gamma}^i/g^{ii}) = 0$ for all $j \neq i$ i.e., to $\hat{\Gamma}^i = g^{ii}\xi_i(q^i)$ (i n.s.). By definition of modified contracted Christoffel symbol (2.7), since the coordinates are orthogonal, we get $\Gamma_i - 2\partial_i \ln R = \xi_i(q^i)$, that is (4.14). The differential system is integrable in orthogonal coordinates satisfying (4.11). Indeed, a straightforward calculation shows that

$$\partial_j \Gamma_i = \partial_i \Gamma_j \Leftrightarrow \partial_{ij}^2 \ln g^{jj} = \partial_{ij}^2 \ln g^{ii} \Leftrightarrow \frac{S_{ij}(g^{jj})}{g^{jj}} = \frac{S_{ij}(g^{ii})}{g^{ii}}.$$

□

Remark 28. By using (4.14) we can write $\Delta R/R$ (included in the modified potential U) in terms of the contracted Christoffel symbols Γ_i as

$$\frac{\Delta R}{R} = \frac{1}{4}g^{ii}(2\partial_i \Gamma_i - \Gamma_i^2 + \xi_i^2 - 2\partial_i \xi_i). \quad (4.15)$$

We shortly recall some definitions arising from the theory of separation of geodesic Hamilton-Jacobi equation (see [4]).

Definition 29. Orthogonal coordinates (q^i) are *separable* if the metric g^{ii} is a *Stäckel metric* i.e. it is a row of the inverse of a regular matrix $S = (\varphi_i^{(j)})$ (*Stäckel matrix*) whose elements depend on the coordinate corresponding to the lower index only. Orthogonal coordinates (q^i) are *conformal separable* if the metric g^{ii} is a *conformal Stäckel metric* i.e., there exists a function Λ such that g^{ii}/Λ is a Stäckel metric. A function f is a *pseudo-Stäckel factor* (resp. *Stäckel factor*), if it can be written as $f = g^{ii}\phi_i(q^i)$, where (g^{ii}) is a conformal Stäckel metric (resp. Stäckel metric).

Theorem 30. *Necessary and sufficient conditions for the FER-separation of (1.1) in a given coordinate system (q^i) (under the assumption $g^{ii} \neq 0 \forall i$) are:*

- (1) *the coordinates are orthogonal;*
- (2) *the coordinates are conformal separable;*
- (3) *the function*

$$\frac{2}{\hbar^2}(E - V) + \frac{1}{4}g^{ii}(2\partial_i \Gamma_i - \Gamma_i^2)$$

is a pseudo-Stäckel factor. In this case R is any solution of equations (4.14).

Proof. By Proposition 22, we have that coordinates are necessarily orthogonal. Moreover, by Proposition 25 in orthogonal coordinates FER-separation occurs if and only if conditions (4.10), (4.11) and (4.12) hold. Equations (4.11) means

that the orthogonal coordinates q^i are conformal separable coordinates, condition (4.12) means that $U - \frac{2}{\hbar^2}E$ is a pseudo-Stäckel factor (see [4]) and, by Proposition 27, Eq. (4.14) determines R up to separated factors. By (4.15), we have that we can replace $U - \frac{2}{\hbar^2}E$ by the function $\frac{2}{\hbar^2}(E - V) + \frac{1}{4}g^{ii}(\partial_i\Gamma_i - \frac{1}{2}\Gamma_i^2)$, disregarding the term $\frac{1}{8}g^{ii}\theta_i$ which is a pseudo-Stäckel factor for any choice of ξ_i in (4.14). \square

Remark 31. In the ordinary separation for Schrödinger equation, condition (3) is split into the compatibility condition for the potential ($V = g^{ii}\theta_i(q^i)$) and the Robertson condition ($\partial_i\Gamma_j = 0$). Moreover, the coordinates are in this case necessarily separable, while in the case of FER-separation conformal separable coordinates are also allowed.

Remark 32. For the Laplace equation, condition (3) of Theorem 30 means that $\frac{1}{4}g^{hh}(2\partial_h\Gamma_h - \Gamma_h^2)$ is a pseudo-Stäckel factor, that is

$$\exists \theta_i(q^i) \mid \frac{g^{hh}}{4}(2\partial_h\Gamma_h - \Gamma_h^2) = g^{ii}\theta_i(q^i). \quad (4.16)$$

We remark that this condition in general does not imply (see [3]),

$$2\partial_i\Gamma_i - \Gamma_i^2 = 4\theta_i(q^i). \quad \forall i \quad (4.17)$$

For example toroidal coordinates (see Section 5) satisfy (4.16) since $g^{hh}(2\partial_h\Gamma_h - \Gamma_h^2) = g^{33}$, but they do not satisfy (4.17). Moreover, even if the (q^i) are separable, (4.16) does not imply the Robertson condition $\partial_i\Gamma_j = 0$ (by (4.14) Robertson condition implies that R is a separated function and R -separation is then called *trivial* [10]). A counterexample of that is given by the conformally flat metric allowing non trivial R -separation in [8]. In [13] condition (4.17) is linked to the fact that symmetry operators can be put in the reduced form.

Proposition 33. *If (q^i) are FER-separable coordinates for (1.1) for two values of the energy $E_1 \neq E_2$, then (q^i) are separable and allow R -separation for all values of the energy.*

Proof. If (4.12) holds for both E_1 and E_2 , then $S_{ij}(g^{kk}) = 0$, $k = 1 \dots n$ and (4.12) hold for all $E \in \mathbb{R}$. \square

4.1 Separated equations

If q^i are conformal separable coordinates for the orthogonal metric $\mathbf{G} = (g^{ii})$, then for any pseudo-Stäckel factor f we have that (g^{ii}/f) is a Stäckel metric. Hence, in coordinates allowing FER-separation we have that the conformal metric $\bar{\mathbf{G}}$ with components

$$\bar{g}^{jj} = \frac{g^{jj}}{\frac{2}{\hbar^2}E - U} \quad (4.18)$$

is a Stäckel metric and that Eq. (2.5) is equivalent to

$$\bar{g}^{ii}(u_{ii} + u_i^2 - \xi_i u_i) = -1, \quad (4.19)$$

for any choice of the functions $\xi_i(q^i)$. In order to integrate Eq. (4.19) by separation of variables, it should be considered as the n -th equation of the system

$$\varphi_{(j)}^i(u_{ii} + u_i^2 - \xi_i u_i) = a_j, \quad (a_n = -1)$$

where $\varphi_{(j)}^i$ is the inverse of a Stäckel matrix associated with the Stäckel metric $\bar{\mathbf{G}}$ and (a_1, \dots, a_n) are real constants. By inverting this system, we get the separated equations

$$u_{ii} + u_i^2 - \xi_i u_i = \sum_{\alpha=1}^{n-1} a_\alpha \varphi_i^{(\alpha)} - \varphi_i^{(n)}, \quad (4.20)$$

corresponding by using (2.10) to the Riccati equations for the separated factors ϕ_i

$$\phi_i'' - \xi_i \phi_i' - \varphi_i^{(j)} a_j \phi_i = 0, \quad (a_n = -1). \quad (4.21)$$

Being R locally determined (up to separated factors) by Eq. (4.14), it is evident that we always can choose $\xi_i = 0$ for $i = 1, \dots, n$ so that (4.14) becomes

$$2\partial_i \ln R = \Gamma_i. \quad (4.22)$$

It follows that

Proposition 34. *In FER-separable coordinates, by choosing R satisfying (4.22), separated equations (4.20), (4.21) have the canonical form*

$$\begin{aligned} u_{ii} + u_i^2 &= a_j \varphi_i^{(j)}, \\ \phi_i'' &= \varphi_i^{(j)} a_j \phi_i. \end{aligned}$$

Remark 35. Even if they do not explicitly appear in the separated equations, the potential V and the value E are contained in the components Stäckel metric $[\varphi_i^{(j)}]$

Remark 36. The above described method of separating the variables gives rise to two kinds of constants in the separated solutions: the $n-1$ constants a_j ($j = 1, \dots, n-1$) of Eq. (4.21) that we call separation constants and the integration constants of Eq. (4.21). Even if the 2nd order Eq. (4.21) give rise to $2n$ constants, n of them are inessential constant factors of the ϕ_i , irrelevant for our purposes as explained at the beginning of the Section. Therefore, there are only n non-trivial integration constants ($b_i = (\phi_i'/\phi_i)_{q_0}$) which, together with the $n-1$ (a_j), form the set of $2n-1$ constants satisfying the completeness condition (4.2). The relation between the constants (a_j, b_i) and the constants (b_i, k_j) introduced in Remark 20 with $(k_j) = (\phi_j''/\phi_j)_{q_0}$ is given by (4.21) evaluated in the initial point q_0 .

In the following subsections, we shall see that, in analogy with the ordinary separation of the Schrödinger equation (see [10, 2, 3] and references therein), the separation constants are in fact the eigenvalues of n second-order pairwise-commuting conformal symmetry operators of the equation related to quadratic first-integrals in involution of an associated Hamilton-Jacobi equation.

4.2 Conformal Killing Tensors and FER-separation

Fixed-Energy separation of (2.5) is characterized by the existence of CKTs of the metric \mathbf{G} in conformal involution with common eigenvectors (see [4]). Indeed, conformal separable coordinates are associated with n symmetric 2-tensors $\mathbf{K}_1, \dots, \mathbf{K}_n = \bar{\mathbf{G}}$ which are Killing tensors with respect to the metric $\bar{\mathbf{G}}$ (4.18), simultaneously diagonalized in the (q^i) , and with contravariant components

$$K_j^{ii} = \varphi_{(j)}^i, \quad K_j^{ih} = 0, \quad \text{for } i \neq h. \quad (4.23)$$

Let us consider the cotangent bundle T^*Q with canonical coordinates (q^i, p_i) and Poisson brackets of functions A, B on T^*Q defined by

$$\{A, B\} = \sum_{i=1}^n \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q^i} - \frac{\partial A}{\partial q^i} \frac{\partial B}{\partial p_i}.$$

Let us construct the quadratic polynomials in the momenta associated with (\mathbf{K}_i)

$$P_{K_h} = K_h^{ij} p_i p_j \quad h \neq n, \quad P_{K_n} = \bar{g}^{ij} p_i p_j. \quad (4.24)$$

We have that [12, 4] the functions P_{K_h} defined by (4.24) and (4.23) satisfy for $h, j = 1, \dots, n$:

$$\{P_{K_h}, P_{K_j}\} = 0, \quad (4.25)$$

i.e., P_{K_h} are pairwise in involution first integrals of the geodesic Hamiltonian P_{K_n} , and the geodesic Hamilton-Jacobi equation $\bar{g}^{ij} p_i p_j = h$ is separable in the (q^i) . Hence, we get

Proposition 37. *An intrinsic necessary condition for the existence of FER-separable coordinates for the Schrödinger equation (1.1) is that there exist $n - 1$ CKTs $\mathbf{K}_1, \dots, \mathbf{K}_{n-1}$ such that (i) $\mathbf{K}_1, \dots, \mathbf{K}_{n-1}, \mathbf{G}$ are linearly independent, (ii) $\mathbf{K}_1, \dots, \mathbf{K}_{n-1}$ have common eigenvectors, and (iii) Eq. (4.25) is satisfied.*

4.3 Symmetry operators

Starting from separated equations (4.20) and (4.21) we build conformal symmetry operators of (1.1). Interpreting the left-hand side of (4.20) as the results of n differential operators acting on u ,

$$u \mapsto \varphi_{(j)}^i (u_{ii} + u_i^2 - \xi_i u_i), \quad (4.26)$$

and inserting (2.10), (4.14), (2.2) in (4.26), we get n operators H_j on ψ defined by

$$H_j\psi = \Delta_j\psi - \frac{1}{R}\Delta_j R\psi, \quad (4.27)$$

where

$$\Delta_j: \psi \mapsto \varphi_{(j)}^i (\partial_{ii}^2 \psi - \Gamma_i \partial_i \psi) = \varphi_{(j)}^i \delta_i \psi, \quad \delta_i: \psi \mapsto \partial_{ii}^2 \psi - \Gamma_i \partial_i \psi. \quad (4.28)$$

For $j = n$ we have $\Delta_n = \Delta/(\frac{2}{\hbar^2}E - U)$ and for $a_n = -1$, $H_n\psi = a_n\psi$ is equivalent to the Schrödinger equation (1.1). By Proposition 27, since $\varphi_{(j)}^i/\bar{g}^{ii}$ are the eigenvalues λ_j^i w.r. to $\bar{\mathbf{G}}$ of n diagonalized KT's of $\bar{\mathbf{G}}$, defined by

$$K_{(j)}^{ii} = \varphi_{(j)}^i = \lambda_j^i \bar{g}^{ii},$$

and since the λ_j^h satisfy the following intrinsic Killing-Eisenhart equations (see [6, 12, 4])

$$\partial_i \lambda_j^h = (\lambda_j^i - \lambda_j^h) \partial_i \log \bar{g}^{hh},$$

a direct computation shows that

Proposition 38. *Let (q^i) be orthogonal conformal separable coordinates and (\mathbf{K}_j) be n independent KT of the conformal metric $\bar{\mathbf{G}}$ (4.18) in involution and simultaneously diagonalized ($K_j^{ih} = \delta^{ih} \varphi_j^i$), with $\mathbf{K}_n = \bar{\mathbf{G}}$. Then, the operators H_i pairwise commute i.e., for $j, k = 1, \dots, n$*

$$[H_j, H_k] = H_j H_k - H_k H_j = 0. \quad (4.29)$$

By expanding $[H_i, S]$, where S denotes the Schrödinger operator $S: \psi \mapsto -\Delta\psi + \frac{2}{\hbar^2}V$, by (4.27) and (4.28), we see that H_i are conformal symmetry operators [9] for S . It follows that

Proposition 39. *FER-separable solutions ψ are common eigenvectors of commuting second order conformal symmetry operators for the Schrödinger operator S .*

5 An example: toroidal coordinates on the Euclidean three-space

Let us consider toroidal coordinates $(q^i) = (\eta, \theta, \varphi)$ on the Euclidean three-space \mathbb{E}_3 . These coordinates have been applied also to biophysical systems [14]. The transformations to Cartesian coordinates (x, y, z) are

$$\begin{cases} x = \frac{a \sinh \eta \cos \varphi}{\cosh \eta - \cos \theta}, \\ y = \frac{a \sinh \eta \sin \varphi}{\cosh \eta - \cos \theta}, \\ z = \frac{a \sin \theta}{\cosh \eta - \cos \theta}. \end{cases} \quad a \in \mathbb{R}^+$$

The coordinates hypersurfaces $q^i = \text{const.}$ are toroids, spherical bowls, and half-planes through the z -axis, respectively [17]. The non vanishing contravariant components of the Euclidean metric in the (q^i) are

$$g^{11} = g^{22} = \frac{(\cosh \eta - \cos \theta)^2}{a^2}, \quad g^{33} = \frac{(\cosh \eta - \cos \theta)^2}{a^2 \sinh^2 \eta}.$$

We consider the FER-separation of Schrödinger equation for $E = 0$

$$\Delta \psi - \frac{2}{\hbar^2} V \psi = 0. \quad (5.1)$$

Since for toroidal coordinates we have $g^{hh}(2\partial_h \Gamma_h - \Gamma_h^2) = g^{33}$, which is a Stäckel factor, condition (3) of Theorem 30 provides the form of all possible potentials allowing FER-separation of (5.1)

$$V = (\cosh \eta - \cos \theta)^2 \left(f_1(\eta) + f_2(\theta) + \frac{1}{\sinh^2 \eta} f_3(\varphi) \right),$$

where f_i are arbitrary functions. By integrating (4.14) we get

$$R = \left(\frac{\cosh \eta - \cos \theta}{\sinh \eta} \right)^{\frac{1}{2}} \quad (5.2)$$

for all $\xi_i = 0$ (canonical separated equations), while we get $R = (\cosh \eta - \cos \theta)^{\frac{1}{2}}$ for the choice $\xi_1 = \text{cotanh} \eta$ (non canonical separated equations)) The conformal metric $\bar{g}^{ii} = g^{ii}/\sigma$ with

$$\sigma = (\cosh \eta - \cos \theta)^2 (f_1(\eta) + f_2(\theta) + (\sinh \eta)^{-2} f_3(\varphi))$$

is a Stäckel metric and associated with the Stäckel matrix (depending on V)

$$S = \begin{bmatrix} f_1 & -1 & -\sinh^{-2} \eta \\ f_2 & 1 & 0 \\ f_3 & 0 & 1 \end{bmatrix}.$$

The separated equations are

$$\begin{aligned} \frac{d^2 \phi_1}{d\eta^2} + \text{cotanh} \eta \frac{d\phi_1}{d\eta} + (f_1 - c_2 - c_3(\sinh \eta)^{-2}) \phi_1 &= 0 \\ \frac{d^2 \phi_2}{d\theta^2} + (f_2 + c_2) \phi_2 &= 0 \\ \frac{d^2 \phi_3}{d\varphi^2} + (f_3 + c_3) \phi_3 &= 0 \end{aligned}$$

where the term in $\frac{d\phi_1}{d\eta}$ disappears if R is chosen to be (5.2). Two conformal Killing tensors in involution associated with toroidal coordinates are

$$\mathbf{K}_1 = \partial_\theta \otimes \partial_\theta + f_2 \bar{\mathbf{G}} \quad \mathbf{K}_2 = \partial_\varphi \otimes \partial_\varphi + f_3 \bar{\mathbf{G}}$$

whose components in Cartesian coordinates (disregarding the term proportional to the metric tensor) are

$$\mathbf{K}_1 = \frac{1}{2a^2} \begin{bmatrix} 2x^2z^2 & 2xyz^2 & -(x^2 + y^2 + z^2)xz \\ " & 2z^2y^2 & -(x^2 + y^2 + z^2)yz \\ " & " & (x^2 + y^2 + z^2)^2 \end{bmatrix} \quad \mathbf{K}_2 = \begin{bmatrix} y^2 & -xy & 0 \\ -xy & x^2 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

The research of non trivial examples of FER-separation for a single value $E \neq 0$ in dimension $n > 2$ is in progress.

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